CRYSTAL ENGINEERING APPROACHES FOR DESIGNING AND STRUCTURAL STUDIES OF NEW MULTICOMPONENT SOLIDS

SYNOPSIS

OF THE Ph.D. THESIS TO BE SUBMITTED

TO

MANGALORE UNIVERSITY

FOR THE AWARD OF DEGREE OF

DOCTOR OF PHILOSOPHY

IN

CHEMISTRY

BY

Ms. SRIJANA, P. J

DEPARTMENT OF STUDIES AND RESEARCH IN CHEMISTRY

MANGALORE UNIVERSITY

MANGALAGANGOTHRI-574199

JULY 2025

Name of Candidate : **Ms. Srijana, P. J**

Title of the Thesis : **Crystal Engineering Approaches for Designing and Structural Studies of New Multicomponent Solids**

Name of the Guide : **Prof. B. Narayana**

Name of the Institution : **Department of Studies and Research in Chemistry**
Mangalore University
Mangalagangothri - 574199

Registration No : **MU/EXB/Ph.D./CR.02/Chem./2022-23/E.25 dated 19-04-2022**

Registration Date : **09-09-2019**

Date of Colloquium : **31-12-2024**

The thesis entitled "**Crystal Engineering Approaches for Designing and Structural Studies of New Multicomponent Solids**" has been divided into six chapters

Chapter 1: An overview of crystal engineering and its application in the synthesis of multicomponent solids

Chapter 2: Studies on the supramolecular architecture of two new proton transfer molecular salts of 2-Aminopyridine

Chapter 3: Studies on crystal packing in the multicomponent solids of pyridine derivatives with dicarboxylic acid coformers

3A. 2-Amino-6-methylpyridinium DL-tartrate molecular salt

3B. Comparative studies on cocrystals of succinic acid with 4-Aminopyridine and 4-Acetylpyridine

Chapter 4 An insight on the hydrogen bonding interactions in multicomponent solids derived from Imidazole and Naphazoline

5A. Imidazolium *p*-hydroxybenzoate molecular salt

5B. Naphazolinium-3-nitrobenzoate and Naphazolinium-5-chlorosalicylate salt- cocrystals

Chapter 5: Structural and computational studies on noncovalent interactions in supramolecular assembly of Fluconazole-2-chloro-5-nitrobenzoic acid cocrystal

Chapter 6: Exploring crystal structure and supramolecular architecture of Flunarizine and Meclizine as picrate salts

Chapter 1: An overview of crystal engineering and its application in the synthesis of multicomponent solids

The field of 'Crystal Engineering' involves designing new molecular solid forms with specific properties by systematically altering their intermolecular interactions [1,2]. This process involves breaking down complex solid-state assemblies into supramolecular synthons, which are comprised of complementary functional groups [3]. These compounds are held together by various noncovalent interactions. Hydrogen bonding, a primary directional interaction in organic molecules, plays a crucial role in supporting crystal engineering principles for supramolecular synthesis [4]. Crystal engineering has become popular among both academic and industrial chemists for its ability to tailor the properties of materials for specific applications.

Solid forms, in general categorized into single and multiple components where each solid form exhibits unique physicochemical properties that could significantly impact the purity, solubility, and other characteristics of the same. Single-component solids include amorphous forms and polymorphs whereas multicomponent solids include cocrystals, salts, and pseudopolymorphs. Cocrystals have garnered significant attention in recent years. The definition of a cocrystal has evolved to describe it as "A multicomponent supramolecular crystal structure consisting of two or more molecules combined into the same crystal lattice through noncovalent interactions with a fixed stoichiometric ratio" [5]. The first recognized cocrystal, known as 'quinhydrone,' was synthesized by Friedrich Wöhler in 1844 using benzoquinone and hydroquinone [6]. The concept of developing cocrystals had generated substantial interest, evident from the increasing number of publications and patent applications related to cocrystals in recent years. While the main desired outcome of cocrystallization is the formation of cocrystals, however, an unsuccessful cocrystallization event might result in the formation of different solid forms, including eutectics, polymorphs, coamorphous solids, physical mixtures, salts, solvates, hydrates, and solid solutions [7].

In multicomponent crystals, distinct molecules can form supramolecular assemblies in various ratios. The stoichiometry of these compounds depends not only on their molar ratio but also on the mode of hydrogen bonding interactions. The mode of hydrogen bonding, in turn, is influenced by internal factors including the presence of different hydrogen bonding groups, donor-acceptor ratio, and the shape and conformational flexibility of the components. Since structure and function are intricately linked at the molecular level, structural studies of

multicomponent crystals are instrumental in understanding their chemical and physical properties, which significantly influence their characteristics. So, in order to investigate hydrogen bonding interactions in supramolecular assemblage, and to explore their role in stabilizing crystal structures, the decision was made to synthesize several multicomponent crystals. The primary task in this synthesis is the selection of coformers, as there is no established rule for screening them. Drawing from previous literature and Cambridge Structural Database (CSD) observations, potential candidates capable of forming hydrogen bonds were identified. Various hydrogen bond donors (carboxylic acids) and acceptors (amines/amides) within the molecules were assessed, and molecules with the potential to form multiple hydrogen bonds were chosen [8,9]. This chapter covers the research area and outlines the background and rationale for the proposed Ph.D. thesis.

Research gap

Despite the prevalence of multicomponent solids today, identifying suitable coformers and directing the creation of the desired solid form presents a considerable challenge. Literature surveys highlight the critical role of synthesizing multicomponent solids in enhancing physicochemical properties especially in pharmaceutical sector. Consequently, ample scope remains for exploring new solid forms of APIs and related compounds at a molecular level. These studies are crucial for deepening our grasp of the fundamental principles that lead to pharmaceutical solid forms with advantageous traits. Being the chemist point of view the role of hydrogen bonding in stabilizing the supramolecular assemblies is of interest to design new APIs and compare the experimental findings with modern computational methods. this would enhance the deeper understanding of the basis for the development of multicomponent solid forms which is of importance for application in diverse fields. So, the present work has been proposed with the following objectives;

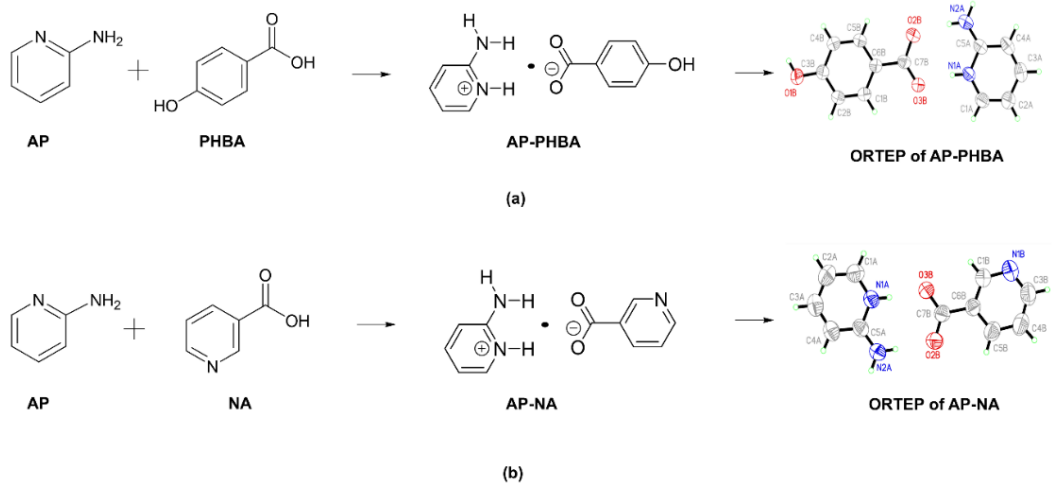
Objectives of the proposed work

- To prepare multicomponent solid forms (cocrystal and salts) of some organic molecules and characterize them using PXRD, TGA/DSC, FT-IR and SCXRD analysis
- To evaluate the intermolecular interactions which stabilize the crystal packing
- To perform Hirshfeld surfaces analysis and other computational analysis of prepared multicomponent solid forms

- To compare the results of SCXRD data with Hirshfeld surfaces analysis
- To investigate the effect of hydrogen bond interactions on the supramolecular network of the compounds

Chapter 2: Studies on the supramolecular architecture of two new proton transfer molecular salts of 2-Aminopyridine

The chapter highlighted the versatility of the acid-pyridine heterosynthon in the construction of molecular salts of 2-aminopyridine (AP) with two distinct coformers. Two new salts of AP i.e., AP-PHBA and AP-NA were synthesized with p-hydroxy benzoic acid (PHBA) and nicotinic acid (NA) respectively and characterized. Both AP-PHBA and AP-NA were crystallized in the monoclinic system with $P2_1/n$ space group. Molecular assemblages in both salts were achieved by combining topology, hydrogen bond connectivity, and graph set analysis. Supramolecular architecture of molecular salts was maintained *via* intermolecular N—H···O, O—H···O and C—H···O hydrogen bonding networks. In both situations, a charge assisted two-point acid-pyridine heterosynthonic ring motif $R_2^2(8)$ was generated by connecting the 2-aminopyridinium cation and carboxylate anion, emphasizing the salt formation. A ribbon synthon was found in both crystals, connecting ring synthon through N2*A*—H2*AB*/*AC*···O3*B* hydrogen bonds with chain motifs $C_2^1(6)$ and $C_2^2(6)$. Two AP molecules were alternately interconnected to two PHBA/NA molecules, resulting in a massive tetramer cage defined by $R_4^4(16)$. The hydroxyl group of PHBA strongly bound the supramolecular aggregation of AP-PHBA via O1*B*—H1*BB*···O2*B* linkages substantiated by a significant O···H (48.4%) contribution to the Hirshfeld surface. In addition, there existed an intermolecular C1*A*—H1*AA*···N1*B* hydrogen bond in AP-NA which interacted with N2*A*—H2*AC*···O3*B* hydrogen bond resulting in $R_4^4(22)$ ring motif, supported by large N···H (12.1%) contribution to the Hirshfeld surface. These results assist in the development of new multicomponent solids of AP with carboxylic acid derivatives based on acid-pyridine synthon as building blocks.



Scheme. 2. The preparation route of (a) AP**-**PHBA and (b) AP**-**NA

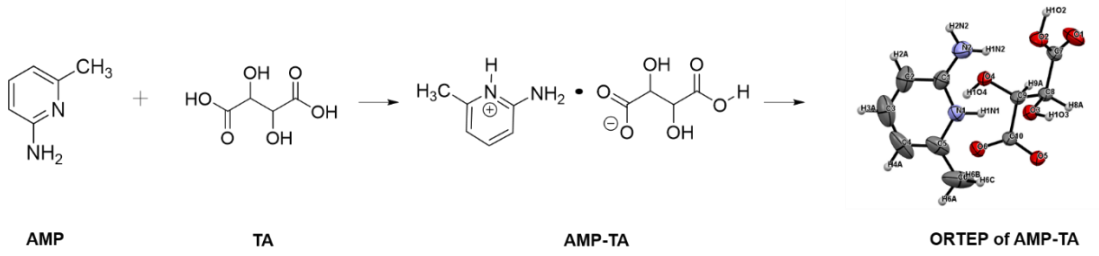
Chapter 3: Studies on crystal packing in the multicomponent solids of pyridine derivatives

3A. 2-Amino-6-methylpyridinium DL-tartrate molecular salt

3B. Comparative studies on cocrystals of succinic acid with 4-aminopyridine and 4-acetylpyridine

3A. 2-Amino-6-methylpyridinium DL-tartrate molecular salt (AMP-TA)

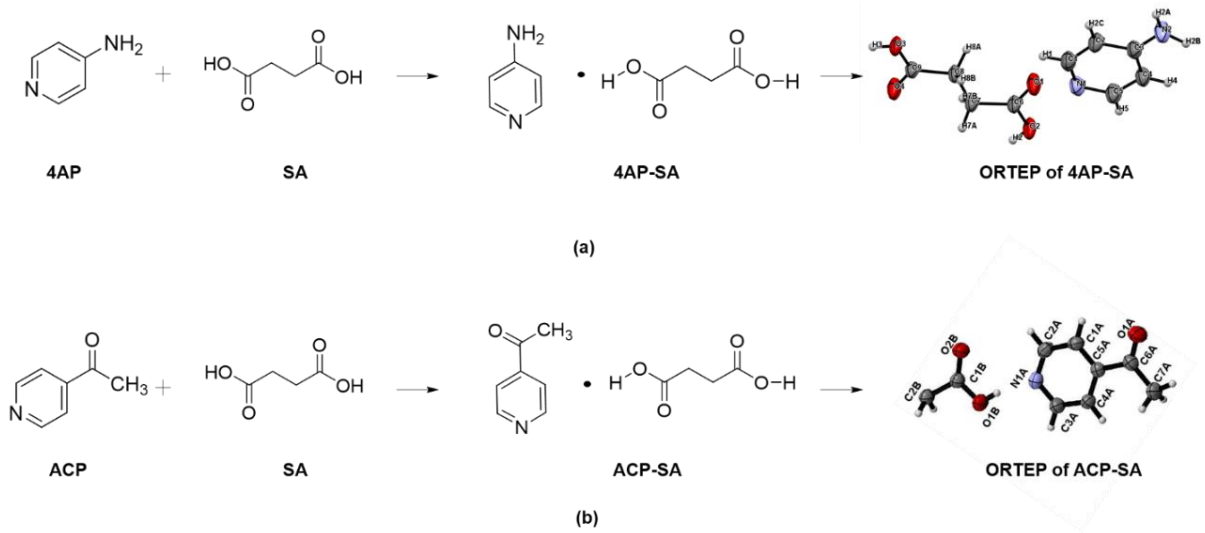
A structural study of new molecular salt of 2-amino-6-methylpyridine (AMP) and DL-tartaric acid (TA) was discussed in this chapter. The formed molecular salt was characterized using spectroscopic and SCXRD techniques. The crystal structure was analyzed in terms of topology, hydrogen bond connectivity, and graph set analysis, revealing a supramolecular architecture stabilized by N−H···O, O−H···O and C−H···O hydrogen bonding networks. These interactions formed ring motifs designated as $R_2^2(9)$, $R_2^2(10)$, $R_2^2(13)$ and S (5), contributing to the overall stability of the AMP−TA assemblage. Furthermore, TA molecules interconnected with one another generating a homosynthonic ring motif with $R_2^2(10)$ and $R_4^2(12)$ through O−H···O hydrogen bonds, were also crucial for maintaining the crystal packing. The importance of O−H···O interactions was further supported by a significant O···H (40.9%) contribution to the Hirshfeld surface. Characteristic FTIR bands for the carboxylate anion (1663 and 1310 cm^{-1}) and C−N^+ (1220 cm^{-1}) confirmed salt formation. These findings provide a basis for designing new multicomponent solids of AMP with carboxylic acid derivatives, utilizing the acid−pyridine synthon as a key building block.



Scheme. 3A. The preparation route of AMP-TA

3B. Comparative studies on cocrystals of succinic acid with 4-aminopyridine and 4-acetylpyridine (4AP-SA and ACP-SA)

In this chapter cocrystals of succinic acid (SA) with two different pyridine derivates was compared. It includes two cocrystals of 4-aminopyridine (4AP) and 4-acetylpyridine (ACP) as coformer. The formation of new solid forms were preliminarily confirmed by FTIR, NMR and thermal analysis. In 4AP-SA, the ring motif is prominent due to hydrogen bonding of SA with amino substituent at the fourth position of pyridine forming $R_2^3(11)$ graph set notation. In the present work acetyl group at the fourth position does not take part in hydrogen bonding with SA molecule. Hence only pyridine N acts as hydrogen bond acceptor forming $R_4^4(22)$ ring motif. As the basicity of substituent increases hydrogen bonding site increases in the case of 4AP-SA cocrystal, while the acetyl group in ACP-SA does not participate in hydrogen bond formation (pK_a of 4AP= 9.1 and ACP= 3.5). Even though the stoichiometry for 4AP-SA is 1:1 the presence of 4-amino group helps in crystal stabilization with multiple interactions. It might be concluded that nature and position of substituent on API play a key role in the crystal packing and stabilization of supramolecular assembly. So, with the help of this study, new design strategies for multicomponent solids of SA with pyridine derivatives can be tested without going through laborious molecular synthesis.



Scheme. 3B. The preparation route of (a) 4AP-SA and (b) ACP-SA

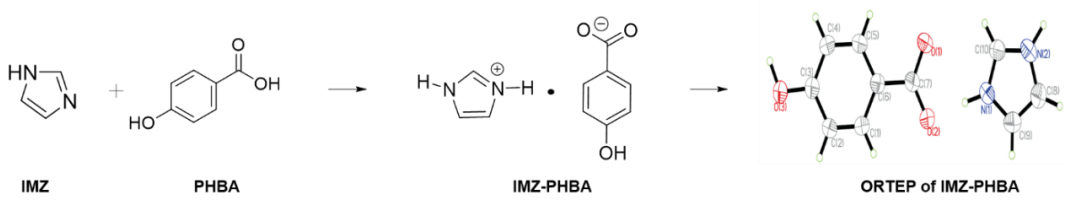
Chapter 4: An insight on the hydrogen bonding interactions in multicomponent solids derived from imidazole and naphazoline

4A. Imidazolium *p*-hydroxybenzoate molecular salt

4B. Naphazolinium 3-nitrobenzoate and naphazolinium 5-chlorosalicylate salt-cocrystals

4A. Imidazolium *p*-hydroxybenzoate (IMZ-PHBA) molecular salt

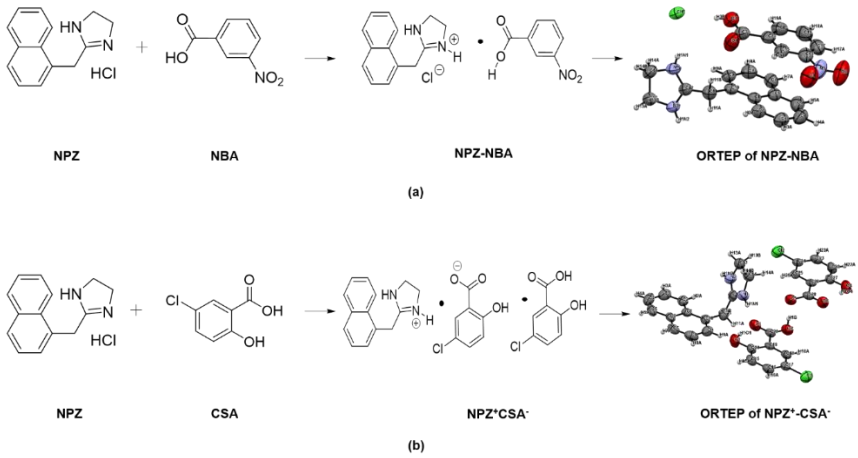
The preparation of IMZ-PHBA molecular salt of imidazole (IMZ) with *p*-hydroxy benzoic acid (PHBA) using the solution evaporation method is discussed in this section. The formed molecular salt was characterized by FTIR, thermal (TGA and DSC) and XRD methods. The IMZ-PHBA was found to crystallized in a monoclinic space group $P2_1/n$, with $Z = 4$. The asymmetric unit of 3D molecular structure revealed the coexistence of IMZ and PHBA ions in 1:1 stoichiometric ratio. The molecular assemblage was achieved by combining topology, hydrogen bond connectivity, and graph set analysis. Supramolecular architecture of IMZ-PHBA was maintained *via* intermolecular N─H···O, O─H···O and C─H···O hydrogen bonding networks. From Hirshfeld surfaces analysis, one could notice that H···H (45.6%) and O···H (23.8%) intercontacts were found to help in stabilizing the supramolecular assembly. The crystal packing and hydrogen bonding were examined with the help of both experimental and Hirshfeld analysis methods.



Scheme. 4A. The preparation route of IMZ-PHBA molecular salt

4B. Naphazolinium 3-nitrobenzoate (NPZ-NBA) and naphazolinium 5-chlorosalicylate (NPZ^{+}-CSA^{-}) salt-cocrystals

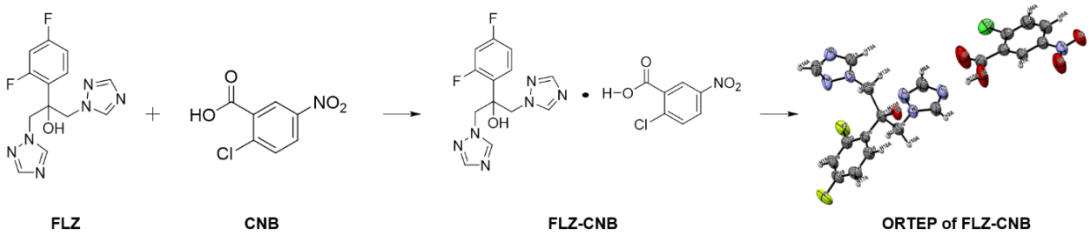
This section reports the structural study of two salt-cocrystals of NPZ using 3-nitrobenzoic acid (NBA) and 5-chlorosalicylic acid (CSA) as coformers. The newly synthesized solids were characterized by different analytical techniques and computational methods. The cocrystallization of NPZ with coformers yielded NPZ-NBA and NPZ^{+}-CSA^{-} salt-cocrystals in a monoclinic lattice. The exchange of proton between NPZ and CSA molecules along with one neutral CSA molecule was identified in the crystal packing. Supramolecular architecture of NPZ^{+}-CSA^{-} was maintained *via* intermolecular N—H···O, C—H···O and intramolecular O—H···O hydrogen bonding networks resulting in $R_3^2(9)$ and S(6) ring motifs respectively. But in NPZ-NBA, the NPZ was bridged to NBA molecule via chloride ion with N1—H1N1···Cl1 and O3—H3B···Cl1 and C11—H11B···O4 interactions, thereby forming a cage with $R_3^2(10)$ ring motif. This was supported by the significant contribution of O···H (23.9%) and H···Cl (10.4%) in the 2D fingerprint plot. With the help of Hirshfeld surfaces, the prominent intermolecular interactions and π···π stacking which contributed to the structural stability of crystals were recognized.



Scheme. 4B. The preparation route of (a) NPZ-NBA and (b) NPZ^{+}-CSA^{-}

Chapter 5: Structural and computational studies on noncovalent interactions in supramolecular assembly of fluconazole-2-chloro-5-nitrobenzoic acid cocrystal (FLZ-CNB)

This part elucidates the synthesis of FLZ-CNB (1:1) cocrystal using the solution method and characterized by FTIR, thermal (TGA and DSC) and XRD methods. The 3D molecular structure comprised one molecule each of fluconazole (FLZ) and 2-chloro-5-nitrobenzoic acid (CNB) in its asymmetric unit. The cocrystal FLZ-CNB was crystallized in triclinic P-1 space group with a=7.2424(6) Å, b=9.9055(8) Å, c=14.9087(12) Å, α=82.540(3)°, β=85.656(3)°, γ=75.564(3)°, volume = 1025.96(15) $Å^3$ and Z=2. The supramolecular architecture of FLZ-CNB was maintained via classical hydrogen bonding and nonclassical interactions. Further, there exists a dimerization of O5—H1···N7 forming a loop $R_2^2(14)$. Another dimer was observed between FLZ molecules through C16—H16*A*···N4 and C17—H17*A*···F2 hydrogen bonds, establishing a distinctive ring motif $R_2^2(11)$. In addition, crystal packing was quantified using computational methods including MESP map, AIMA, NBO, NCI and Hirshfeld surfaces analysis. In the crystal packing, intercontacts H···H (21.7 %), O···H (21.5 %) and O···H (12.1 %) contribute more towards Hirshfeld surfaces. So, this study provides the platform for making cocrystal FLZ-CNB which may improve the physicochemical properties of the FLZ molecule and hence the expansion of new pharmaceutical solid forms.

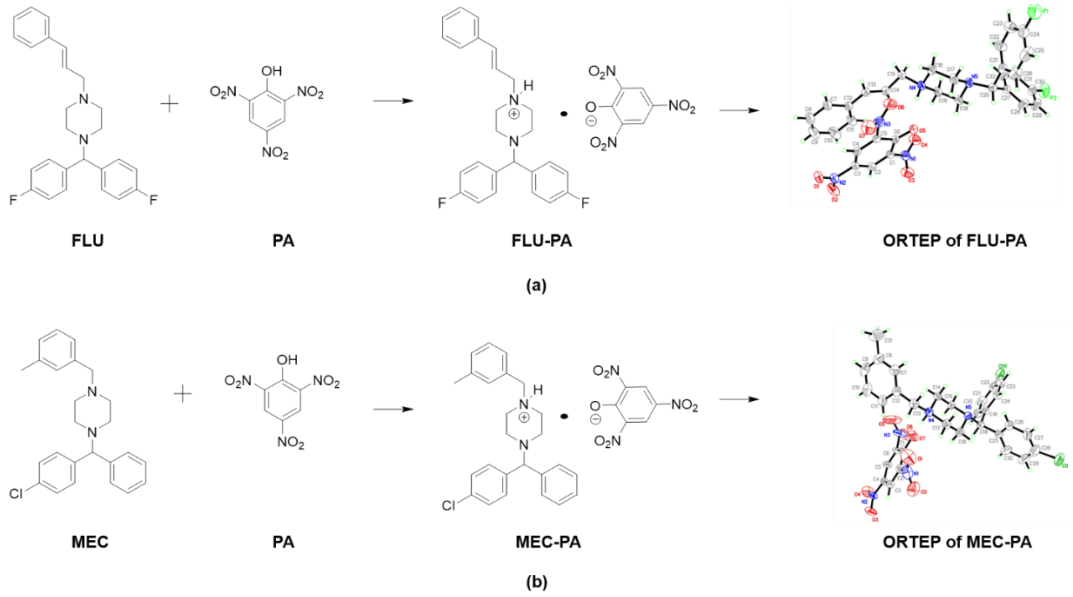


Scheme. 5. The preparation route of FLZ-CNB cocrystal

Chapter 6: Exploring crystal structure and supramolecular architecture of flunarizine and meclizine as picrate salts

This section includes the supramolecular study of salts of flunarizine and meclizine, the typical antihistaminic drugs that fall under BCS class II. The structural and analytical characterization of newly synthesized two molecular salts of flunarizine (FLU) and meclizine (MEC) with picric acid (PA) have been envisaged. The bulk phase purity and homogeneity of the material were confirmed by PXRD analysis. By using FTIR and NMR analysis, the functional groups present in both salts were identified. The melting point of the molecular salts (FLU-PA: 307

°C and MEC-PA: 245.6 °C) was found to be higher than the respective APIs. The single crystal X-ray diffraction analysis revealed the crystal structure of FLU-PA and MEC-PA, which was in monoclinic crystal system. Variations in bond lengths and bond angles confirmed the proton transfer from PA molecule to FLU/MEC molecule. Both molecular salts were discovered to have bifurcated N−H···O linkages between the FLU/MEC cation and picrate anions. From Hirshfeld surfaces analysis, one could notice that H···H, O···H, and C···H intercontacts were found to help in stabilizing the supramolecular assembly.



Scheme. 6. Synthetic pathway of the (a) FLU-PA and (b) MEC-PA

Research outcome

- Eleven new multicomponent solids (AP-PHBA, AP-NA, 4AP-SA, ACP-SA, AMP-TA, IMZ-PHBA, NPZ-NBA, NPZ^{+}-CSA^{-}, FLZ-CNB, FLU-PA and MEC-PA) composed of pharmaceutically important and allied molecules were prepared
- All the new solid forms were preliminarily characterized by FTIR, PXRD, TGA/DSC and NMR analysis
- The single crystal X-ray diffraction data were collected, and structural refinements were performed to confirm the formation of multicomponent solids
- The intermolecular interactions and their effect on stabilizing the supramolecular assemblage of all prepared molecular solids were explored
- Hirshfeld surfaces and other computational analyses were performed which supported the existence of noncovalent interactions within the crystal packing

References

[1] G.R. Desiraju, Crystal engineering: Structure, property and beyond, IUCrJ. 4 (2017) 710–711. https://doi.org/10.1107/S2052252517014853.

[2] G.R. Desiraju, Crystal engineering and IUCrJ, IUCrJ. 3 (2016) 1–2. https://doi.org/10.1107/S2052252515024100.

[3] G.R. Desiraju, Supramolecular Synthon in Crystal Engineering-A New Organic Synthesis, Angew. Chem. Int. Ed. 34 (1995) 2311–2327. https://doi.org/10.1002/3527605746.ch19.

[4] E.R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A.J. Cohen, W. Yang, Revealing noncovalent interactions, J. Am. Chem. Soc. 132 (2010) 6498–6506. https://doi.org/10.1021/ja100936w.

[5] F. Lara-Ochoa, G. Espinosa-Pérez, Cocrystals definitions, Supramol. Chem. 19 (2007) 553–557. https://doi.org/10.1080/10610270701501652.

[6] G.R. Desiraju, Crystal and co-crystal, CrystEngComm. 5 (2003) 466–467. https://doi.org/10.1039/b313552g.

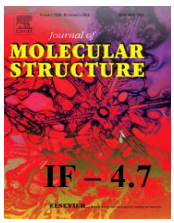
[7] S. Aitipamula, R. Banerjee, A.K. Bansal, K. Biradha, M.L. Cheney, A.R. Choudhury, G.R. Desiraju, A.G. Dikundwar, R. Dubey, N. Duggirala, P.P. Ghogale, S. Ghosh, P.K. Goswami, N.R. Goud, R.R.K.R. Jetti, P. Karpinski, P. Kaushik, D. Kumar, V. Kumar, B. Moulton, A. Mukherjee, G. Mukherjee, A.S. Myerson, V. Puri, A. Ramanan, T. Rajamannar, C.M. Reddy, N. Rodriguez-hornedo, R.D. Rogers, T.N.G. Row, P. Sanphui, N. Shan, G. Shete, A. Singh, C.C. Sun, J.A. Swift, R. Thaimattam, T.S. Thakur, R.K. Thaper, S.P. Thomas, S. Tothadi, V.R. Vangala, N. Variankaval, P. Vishweshwar, D.R. Weyna, M.J. Zaworotko, Polymorphs, Salts, and Cocrystals: What ' s in a Name?, Cryst. Growth Des. 12 (2012) 2147–212. https://doi.org/https://doi.org/10.1021/cg3002948.

[8] T.R. Shattock, K.K. Arora, P. Vishweshwar, M.J. Zaworotko, Hierarchy of supramolecular synthons: Persistent carboxylic acid···pyridine hydrogen bonds in cocrystals that also contain a hydroxyl moiety, Cryst. Growth Des. 8 (2008) 4533–4545. https://doi.org/10.1021/cg800565a.

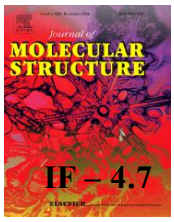
[9] P. Vishweshwar, A. Nangia, V.M. Lynch, Recurrence of Carboxylic Acid - Pyridine Supramolecular Synthon in the Crystal Structures of Some Pyrazinecarboxylic Acids, J. Org. Chem. (2002) 556–565. https://doi.org/10.1021/jo0162484.

List of research papers published in journals and presented in conferences

1. **Srijana, P. J**., Narayana, B., Sarojini, B. K., Ramzi, F. D. B., Quah, C. K., Rajimone, K. J., & Renjith Thomas. (2024). Supramolecular and computational analysis of Fluconazole-2-chloro-5-nitrobenzoic acid cocrystal. *Journal of Molecular Structure*, 1321, 140143. doi: 10.1016/j.molstruc.2024.140143.



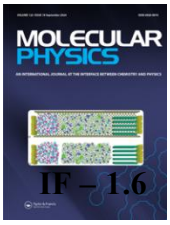
2. **Srijana, P. J**., Narayana, B., Sarojini, B. K., Wong, Q. A., Quah, C. K., & Likhitha, U. (2023). Synthesis and structural studies on the supramolecular architecture of two novel proton transfer molecular salts of 2-aminopyridine. *Journal of Molecular Structure*, 1274, 134426. doi: 10.1016/j.molstruc.2022.134426.



3. **Srijana, P. J**., Karthick, T., Narayana, B., Sarojini, B. K., Wong, Q. A., Quah, C. K., & Likhitha, U. (2024). 4-Acetylpyridine-succinic acid cocrystal: Synthesis, X-ray structure, DFT and Hirshfeld surfaces analysis. *Molecular Crystals and Liquid Crystals*, 768 (5) 47-62. doi: 10.1080/15421406.2023.2300908.

IF – 0.7

4. **Srijana, P. J**., Singh, M., Narayana, B., Sarojini, B. K., Likhitha, U., & Kant, R. (2022). Co-crystallisation of 4-aminopyridine with succinic acid (1:1) : spectroscopic, thermal, crystal structure, DFT/HF calculation and Hirshfeld surface analysis. *Molecular Physics*, 120 (14), e2096143. doi: 10.1080/00268976.2022.2096143.

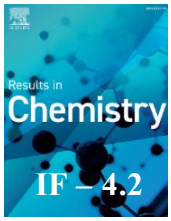


5. **Srijana, P. J**., Narayana, B., Sarojini, B. K., Quah, C. K., Synthesis and structural analysis of succinic acid-4-acetylpyridine cocrystal. International Conference on Functional Materials for Advanced Technology (ICFMAT-1), Department of Physics, Central University of Kerala, January 2-4, 2023.

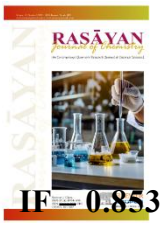
6. **Srijana, P. J**., Narayana, B., Sarojini, B. K., Quah, C. K., Synthesis and structural characterization of Fluconazole-2-chloro-5-nitrobenzoic acid cocrystal. National Conference on Condensed Matter Physics and Applications (CMPA), Department of Physics, MIT, Manipal, on December 14-15, 2023.

List of other publications

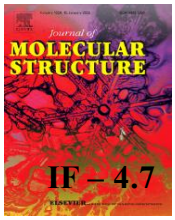
1. Gauthama, B. U., Narayana, B., Sarojini, B. K., **Srijana, P. J**., Kodlady, S. N., Sangappa, Y., Avinash Kudva, & Raghu, S. V. (2024). A hybrid fluorescent probe for the selective detection of divalent Hg^{2+} and trivalent Al^{3+} ions and their biological applications. *Results in Chemistry*, *8*, 101591. doi: 10.1016/j.rechem.2024.101591.



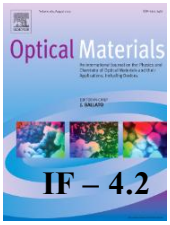
2. Sharma, R., Singh, D., Srijana, P. J., Narayana, B., Sarojini, B. K., Likhitha, U., Murugavel, S., Raj, J. M., & Kant, R. (2024). Cocrystal of 2-amino-6-methyl pyridine with diphenylacetic acid: synthesis, X-ray structure, quantum chemical calculation, Hirshfeld surface analysis and antibacterial activity. *Rasayan Journal of Chemistry*, *17* (4). doi: 10.31788/RJC.2024.1749005.



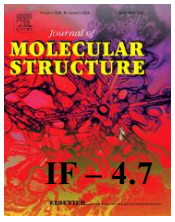
3. Dayananda, B. S., Sarojini, B. K., Wong, Q. A., Quah, C. K., **Srijana, P. J**., & Varma, V. R. (2023). X-aggregation-induced emission in newly fabricated Pullulan/3-Hydroxyflavone derivative composite electrospun nanofiber mat for optical applications. *Journal of Molecular Structure*, *1286*, 135523. doi: 10.1016/j.molstruc.2023.135523.



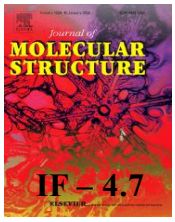
4. Dayananda, B. S., Sarojini, B. K., Wong, Q. A., Quah, C. K., & **Srijana, P. J**. (2023). J-aggregation-induced photoluminescence in electrospun pullulan/2-(2-fluorophenyl)-3-hydroxy-4H-chromen-4-one composite mat for photonic applications. *Optical Materials*, *143*, 114303. doi: 10.1016/j.optmat.2023.114303.



5. Sharma, R., Singh, M., **Srijana, P. J**., Narayana, B., Sarojini, B. K., Likhitha, U., Murugavel, S., Raj, J. M., & Kant, R. (2023). Synthesis, characterization, quantum chemical calculation, Hirshfeld surface analysis and antibacterial activity of a co-crystal of 4-Aminopyridine: p-Hydroxybenzoic acid with a water molecule. *Journal of Molecular Structure*, *1284*, 135309. doi: 10.1016/j.molstruc.2023.135309.

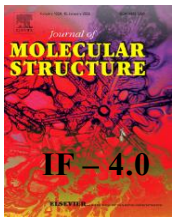


6. Sharma, R., **Srijana, P. J**., Singh, M., Narayana, B., Sarojini, B. K., Likhitha, U., Murugavel, S., Raj, J. M., & Kant, R. (2022). Supramolecular co-crystal of 4-dimethyl aminopyridine with Picric acid (4DMAP: PA): Synthesis, single crystal investigation, HF/DFT

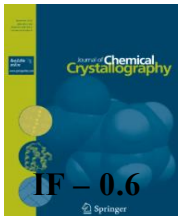


inspection, Hirshfeld surface and antifungal activity. *Journal of Molecular Structure*, *1270*, 133921. doi: 10.1016/j.molstruc.2022.133921.

7. Singh, M., Anthal, S., Srijana, P. J., Narayana, B., Sarojini, B. K., Likhitha, U., & Kant, R. (2022). Novel supramolecular co-crystal of 3-aminobenzoic acid with 4-acetyl-pyridine: Synthesis, X-ray structure, DFT and Hirshfeld surface analysis. *Journal of Molecular Structure*, *1262*, 133061. doi: 10.1016/j.molstruc.2022.133061.



8. Likhitha, U., Narayana, B., Sarojini, B. K., Kumar, S. M., Anup, N., Srijana, P. J., & Yathirajan, H. S. (2022). Stabilization of the DMSO Solvate of 2-Chloro-5-nitrobenzoic acid (Mesalazine Impurity M) by Bifurcated Hydrogen Bonds: Crystallographic, Spectroscopic, Thermal and Computational Studies. *Journal of Chemical Crystallography*, 1-11. doi: 10.1007/s10870-021-00913-1.



Prof. B. Narayana
(Research Guide)

Srijana P. J.
(Research Student)